



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:19 PM GMT

PDB ID : 3CCJ
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2534U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

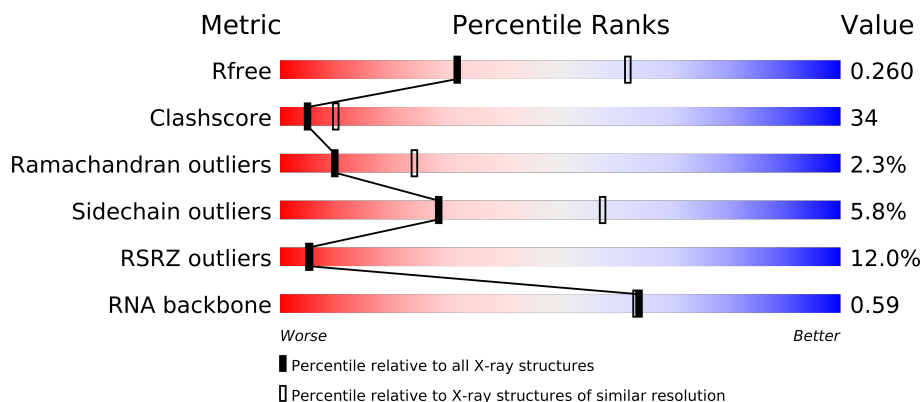
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	

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Mol	Chain	Length	Quality of chain
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8001	-	X
32	MG	0	8008	-	X
32	MG	0	8009	-	X
32	MG	0	8011	-	X
32	MG	0	8022	-	X
32	MG	0	8023	-	X
32	MG	0	8029	-	X
32	MG	0	8030	-	X
32	MG	0	8033	-	X
32	MG	0	8036	-	X
32	MG	0	8037	-	X
32	MG	0	8039	-	X
32	MG	0	8043	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8061	-	X
32	MG	0	8064	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8066	-	X
32	MG	0	8070	-	X
32	MG	0	8071	-	X
32	MG	0	8078	-	X
32	MG	0	8079	-	X
32	MG	0	8081	-	X
32	MG	0	8089	-	X
32	MG	9	8040	-	X
32	MG	9	8074	-	X
32	MG	Y	8077	-	X
33	K	0	8401	-	X
34	NA	0	8501	-	X
34	NA	0	8502	-	X
34	NA	0	8506	-	X
34	NA	0	8508	-	X
34	NA	0	8509	-	X
34	NA	0	8512	-	X
34	NA	0	8514	-	X
34	NA	0	8516	-	X
34	NA	0	8517	-	X
34	NA	0	8518	-	X
34	NA	0	8521	-	X
34	NA	0	8522	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8527	-	X
34	NA	0	8528	-	X
34	NA	0	8530	-	X
34	NA	0	8531	-	X
34	NA	0	8534	-	X
34	NA	0	8535	-	X
34	NA	0	8536	-	X
34	NA	0	8537	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	X
34	NA	0	8545	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8549	-	X
34	NA	0	8551	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8555	-	X
34	NA	0	8556	-	X
34	NA	0	8558	-	X
34	NA	0	8559	-	X
34	NA	0	8560	-	X
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8571	-	X
34	NA	0	8574	-	X
34	NA	B	8552	-	X
34	NA	L	8568	-	X
34	NA	Q	8540	-	X
34	NA	R	8575	-	X
35	CL	0	8805	-	X
35	CL	0	8813	-	X
35	CL	0	8815	-	X
35	CL	0	8822	-	X
35	CL	A	8809	-	X
35	CL	B	8819	-	X
35	CL	J	8816	-	X
35	CL	J	8821	-	X
35	CL	M	8818	-	X
35	CL	N	8807	-	X
35	CL	O	8808	-	X
35	CL	Q	8811	-	X
36	SR	0	8903	-	X
36	SR	0	8904	-	X
36	SR	0	8905	-	X
36	SR	0	8922	-	X
36	SR	0	8924	-	X
36	SR	0	8925	-	X
36	SR	0	8926	-	X
36	SR	0	8931	-	X
36	SR	0	8937	-	X
36	SR	0	8939	-	X
36	SR	0	8941	-	X
36	SR	0	8946	-	X
36	SR	0	8951	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	8957	-	X
36	SR	0	8958	-	X
36	SR	0	8964	-	X
36	SR	0	8969	-	X
36	SR	0	8971	-	X
36	SR	0	8974	-	X
36	SR	0	8979	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8998	-	X
36	SR	0	9000	-	X
36	SR	0	9004	-	X
36	SR	0	9007	-	X
36	SR	9	8980	-	X
36	SR	B	8987	-	X
36	SR	J	8986	-	X
36	SR	R	8912	-	X
37	CD	3	8704	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10872	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	Y	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	2	Total	Mg	0	0
			2	2		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	M	1	Total	K	0	0
			1	1		

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	63	Total	Na	0	0
			63	63		
34	J	1	Total	Na	0	0
			1	1		
34	Q	1	Total	Na	0	0
			1	1		
34	B	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		
34	R	3	Total	Na	0	0
			3	3		
34	9	2	Total	Na	0	0
			2	2		
34	L	1	Total	Na	0	0
			1	1		
34	S	1	Total	Na	0	0
			1	1		
34	M	1	Total	Na	0	0
			1	1		

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	8	Total	Cl	0	0
			8	8		
35	J	4	Total	Cl	0	0
			4	4		
35	Q	1	Total	Cl	0	0
			1	1		
35	B	1	Total	Cl	0	0
			1	1		
35	A	1	Total	Cl	0	0
			1	1		
35	N	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	93	Total 93	Sr 93	0	0
36	J	1	Total 1	Sr 1	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	2	Total 2	Sr 2	0	0
36	2	1	Total 1	Sr 1	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	2	Total 2	Sr 2	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5813	Total O 5813 5813	0	0
38	9	144	Total O 144 144	0	0
38	A	122	Total O 122 122	0	0
38	B	158	Total O 158 158	0	0
38	C	176	Total O 176 176	0	0
38	D	51	Total O 51 51	0	0
38	E	51	Total O 51 51	0	0
38	F	27	Total O 27 27	0	0
38	G	15	Total O 15 15	0	0
38	H	73	Total O 73 73	0	0
38	I	3	Total O 3 3	0	0
38	J	55	Total O 55 55	0	0
38	K	61	Total O 61 61	0	0
38	L	99	Total O 99 99	0	0
38	M	148	Total O 148 148	0	0

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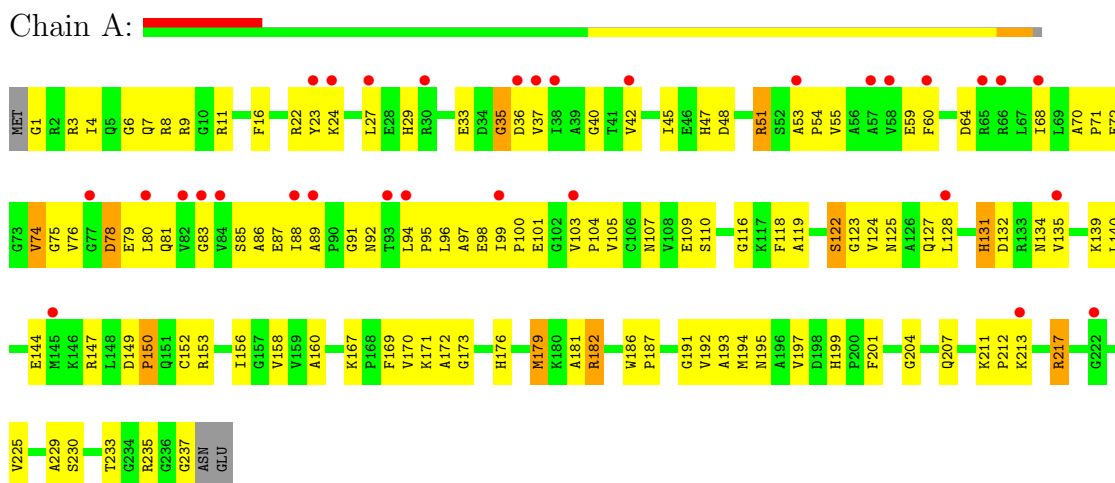
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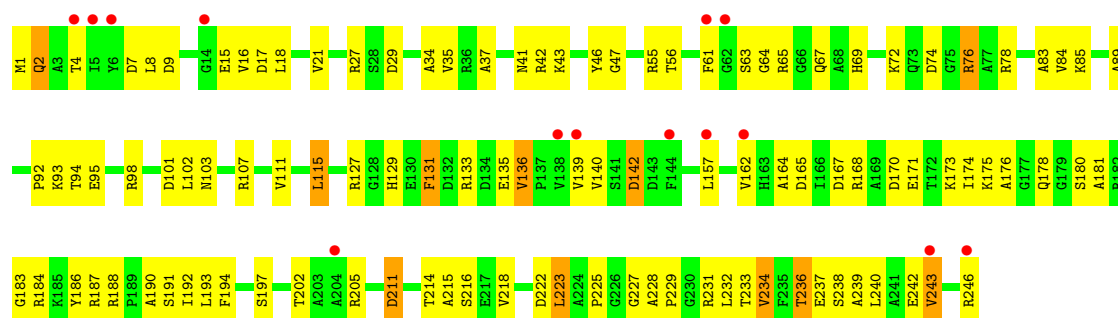
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38	O	42	Total 42	O 42	0	0
38	P	56	Total 56	O 56	0	0
38	Q	58	Total 58	O 58	0	0
38	R	78	Total 78	O 78	0	0
38	S	37	Total 37	O 37	0	0
38	T	41	Total 41	O 41	0	0
38	U	34	Total 34	O 34	0	0
38	V	10	Total 10	O 10	0	0
38	W	71	Total 71	O 71	0	0
38	X	28	Total 28	O 28	0	0
38	Y	102	Total 102	O 102	0	0
38	Z	33	Total 33	O 33	0	0
38	1	53	Total 53	O 53	0	0
38	2	48	Total 48	O 48	0	0
38	3	80	Total 80	O 80	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

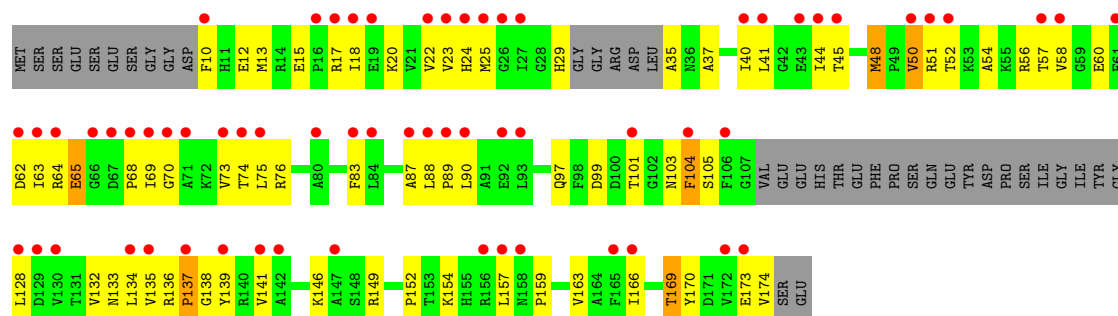
• Molecule 1: 50S ribosomal protein L2P





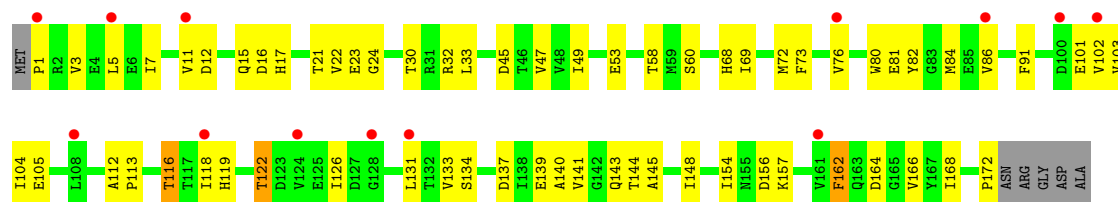
• Molecule 4: 50S ribosomal protein L5P

Chain D:



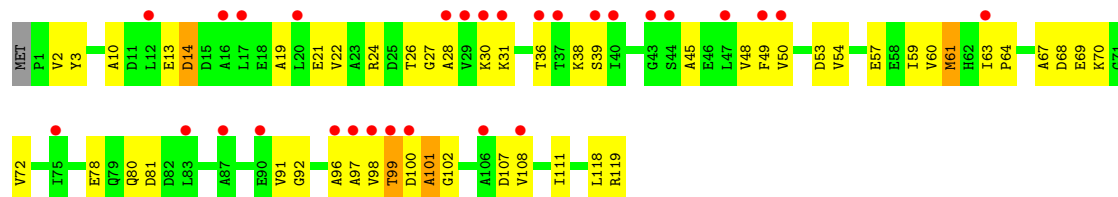
• Molecule 5: 50S ribosomal protein L6P

Chain E:



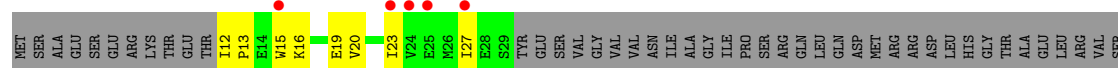
• Molecule 6: 50S ribosomal protein L7Ae

Chain F:



• Molecule 7: 50S ribosomal protein L10E

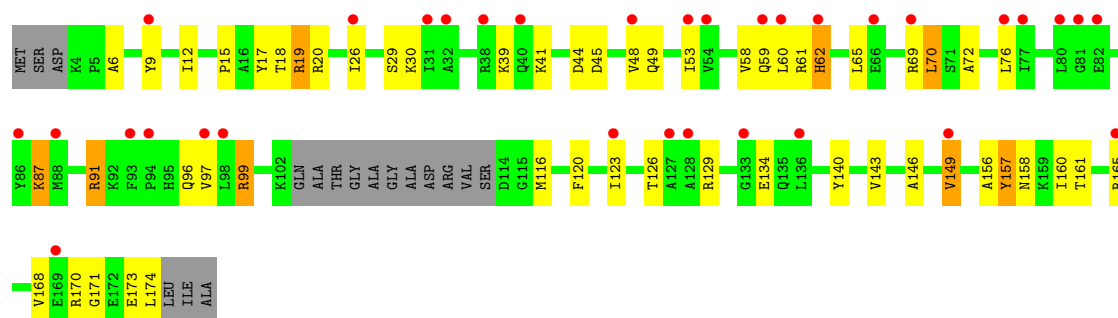
Chain G:





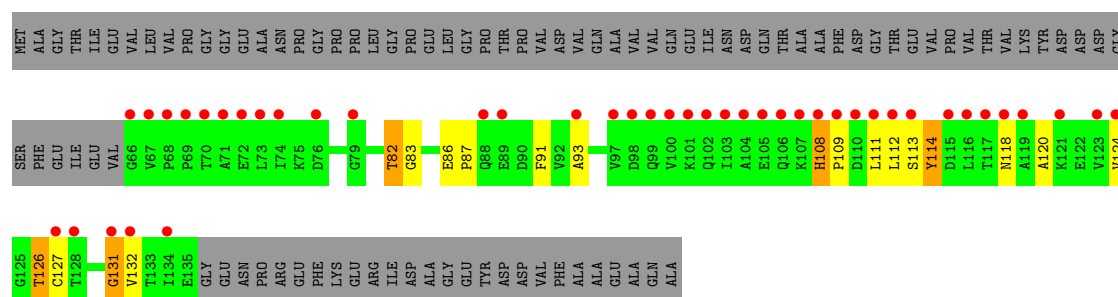
• Molecule 8: 50S ribosomal protein L10e

Chain H:



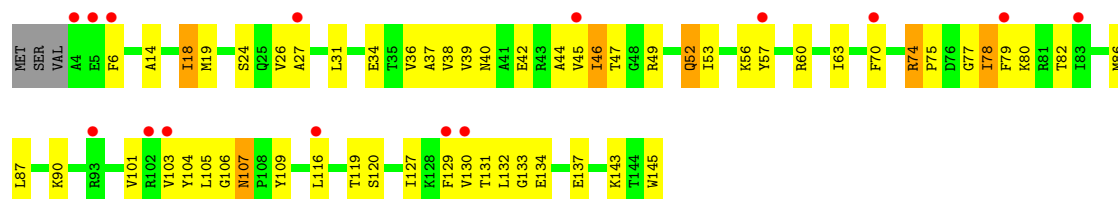
• Molecule 9: 50S ribosomal protein L11P

Chain I:



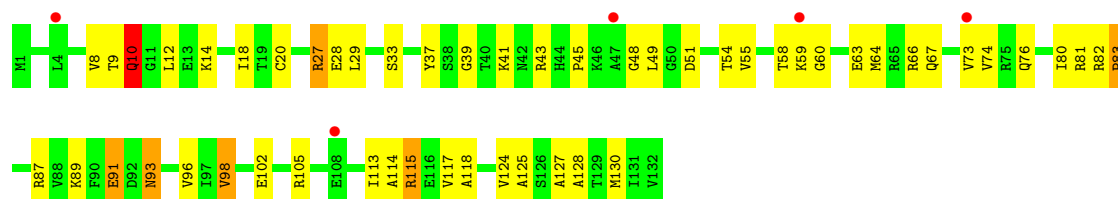
• Molecule 10: 50S ribosomal protein L13P

Chain J:



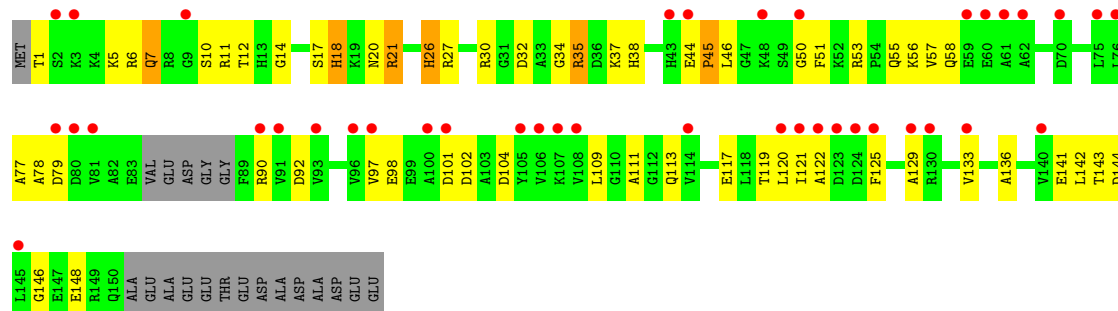
• Molecule 11: 50S ribosomal protein L14P

Chain K: 



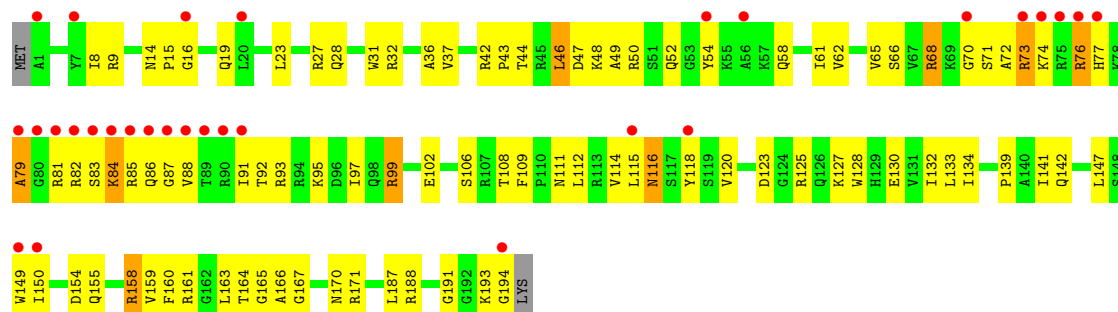
- Molecule 12: 50S ribosomal protein L15P

Chain L: 



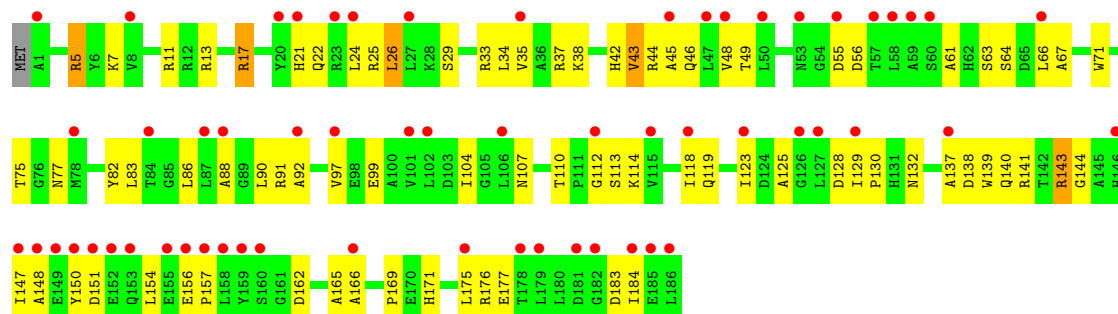
- Molecule 13: 50S ribosomal protein L15e

Chain M: 



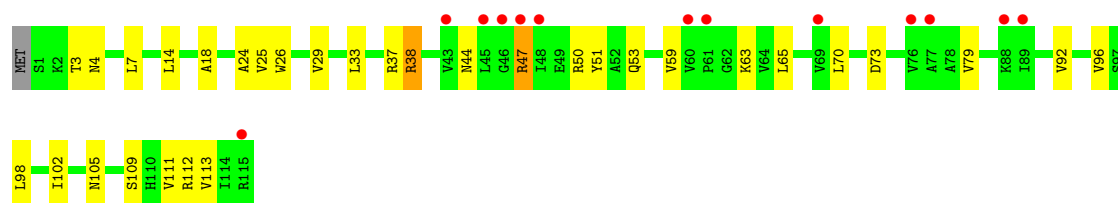
- Molecule 14: 50S ribosomal protein L18P

Chain N: 



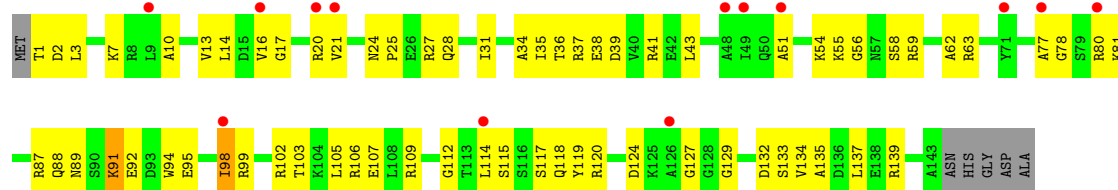
- Molecule 15: 50S ribosomal protein L18e

Chain O: 



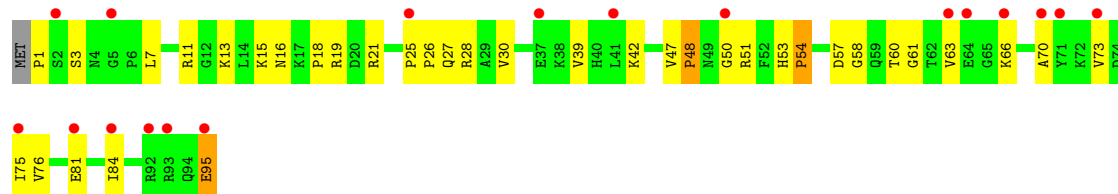
- Molecule 16: 50S ribosomal protein L19e

Chain P:



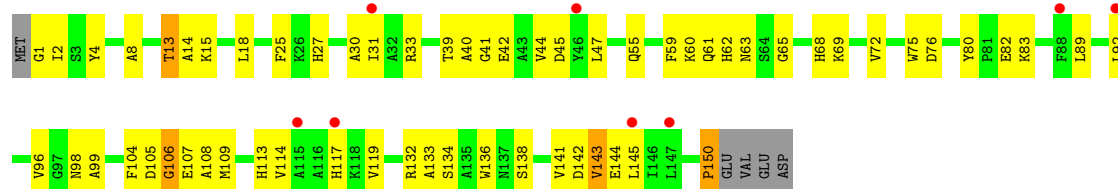
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



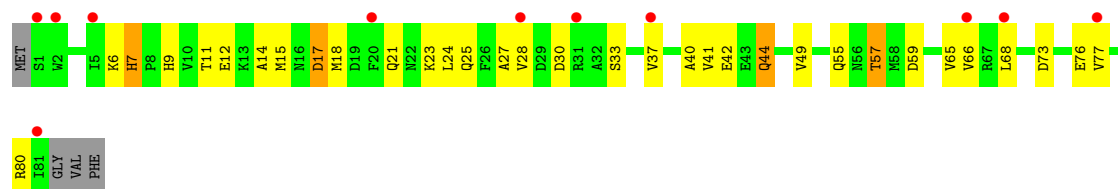
- Molecule 18: 50S ribosomal protein L22P

Chain R:



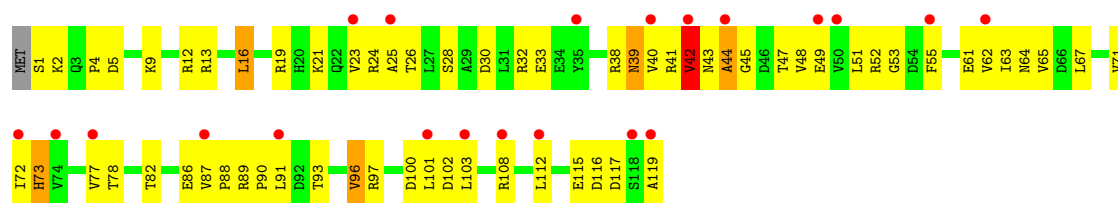
- Molecule 19: 50S ribosomal protein L23P

Chain S:



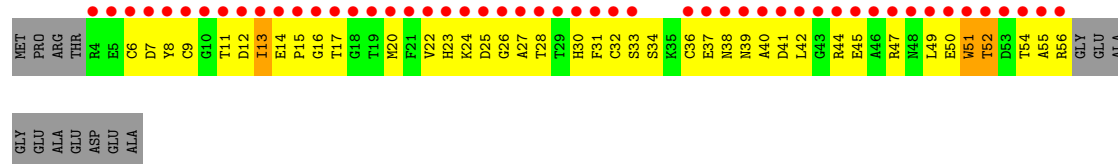
- Molecule 20: 50S ribosomal protein L24P

Chain T:



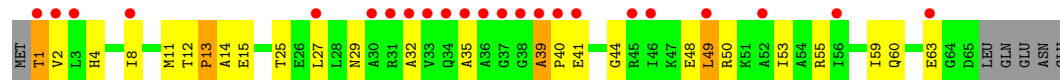
- Molecule 21: 50S ribosomal protein L24e

Chain U:



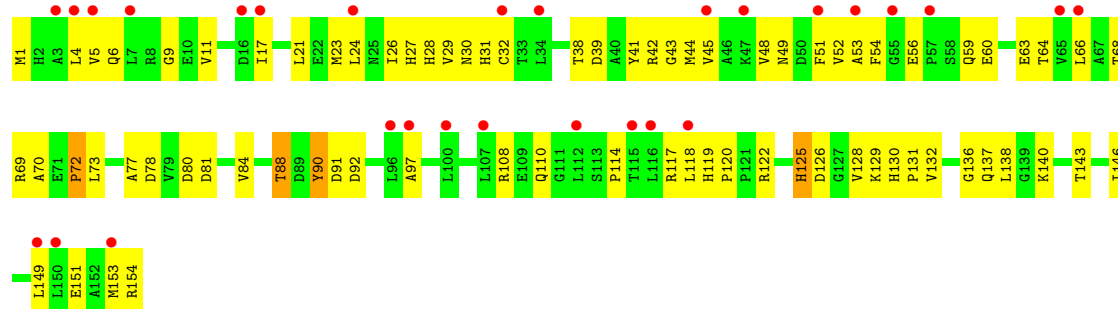
- Molecule 22: 50S ribosomal protein L29P

Chain V:



- Molecule 23: 50S ribosomal protein L30P

Chain W:



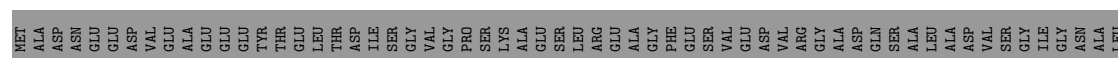
- Molecule 24: 50S ribosomal protein L31e

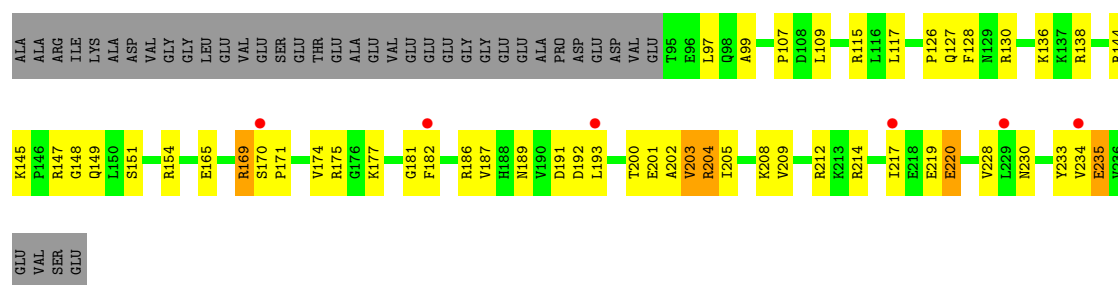
Chain X:



- Molecule 25: 50S ribosomal protein L32e

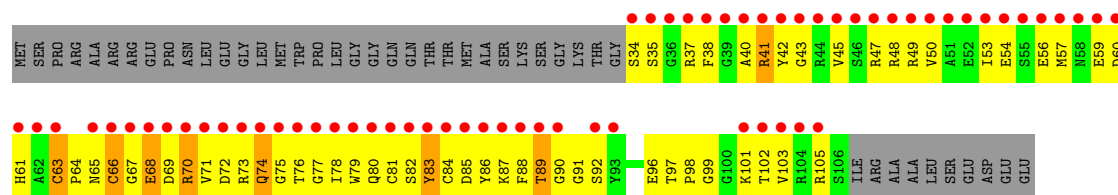
Chain Y:





- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



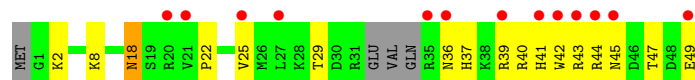
- Molecule 27: 50S ribosomal protein L37e

Chain 1:



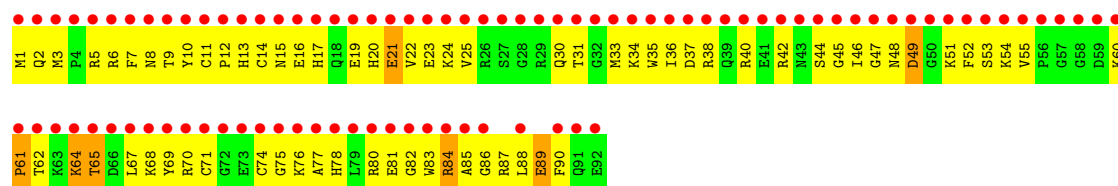
- Molecule 28: 50S ribosomal protein L39e

Chain 2:



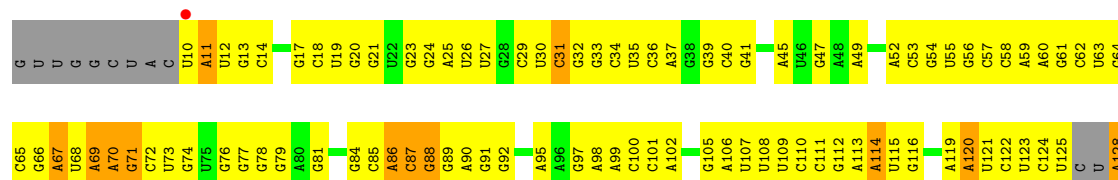
- Molecule 29: 50S ribosomal protein L44E

Chain 3:



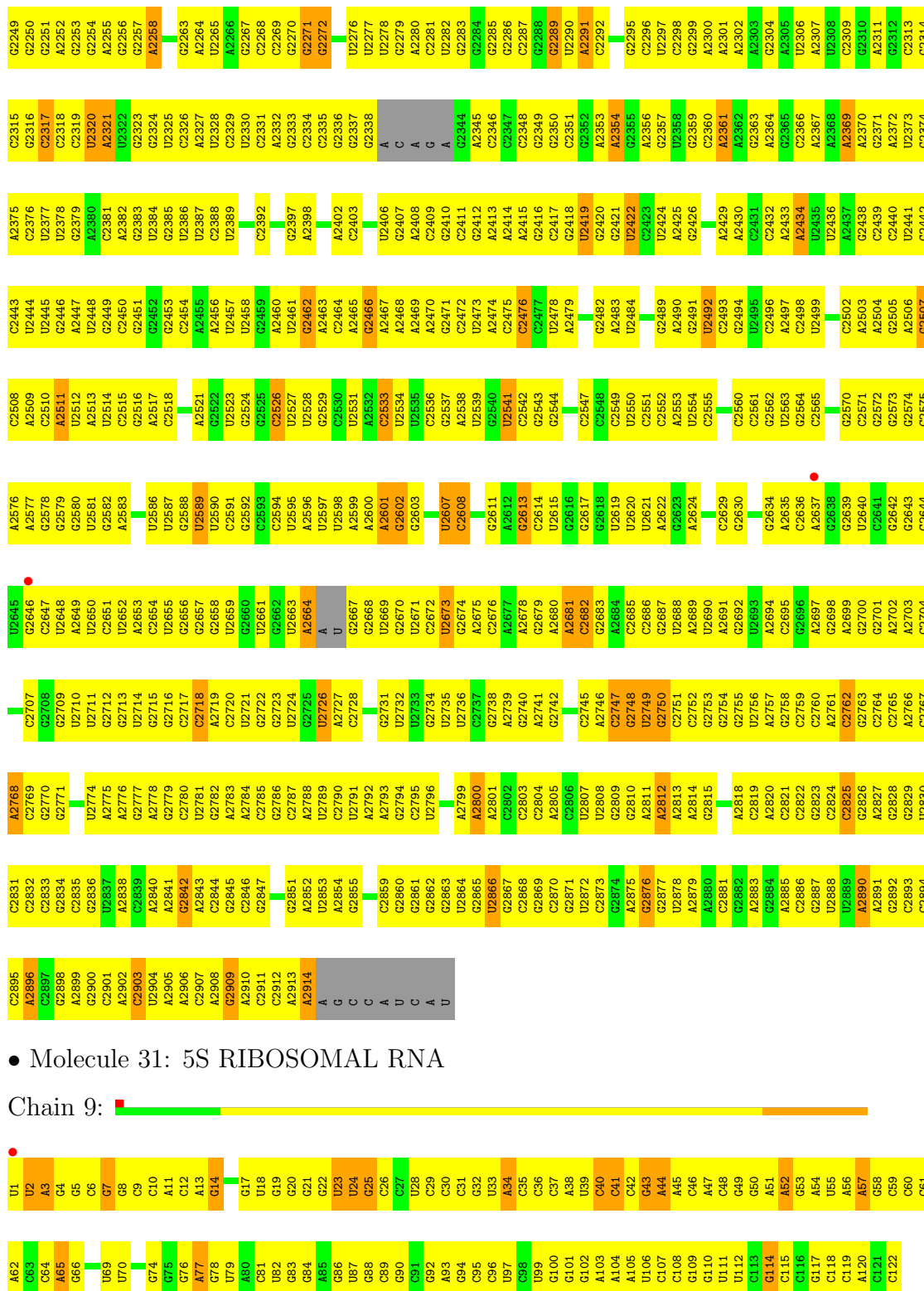
- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:



G1131	G1054	A	G928	U855	A790	U714	G646	U582	A513	G446	G384	A317	C256	A129
A1132	G1055	G	G928	G856	A791	U	U647	C583	G814	A447	C385	U318	G257	C130
G1137	U1056	U	U932	A857	G792	G716	G648	U584	G517	G448	G386	A319	G258	A131
A1057	A1057	C	C933	U858	A793	C717		C585	U517		G387	G320	G259	C195
G1059	G1138	G	C933	C859	U794	C718	G652	C586	A519	C451	G388	A321	G260	G196
C1060	U1139	C	G935	U860	G795	C719	U653	C587	A520	C452	G389	G322	A261	C197
U1141	C1061	C	C936	A861	A796	G720		G588	A521	A453	G390	C323	C136	C136
C1142	U1062	A	C937	U862	G797	G721	G656	U589	U522	U454	U391	G324	U263	C137
G1063	G938	A	G938	U864	G798	G722	G657	A590	G525	A455	U392	U325	U264	U138
C999	U1066	C	A939	A867	G800	G723	G658	G591	G526	A456	G393	A327	G265	U139
C1000	G940	C	G940	A868	G801	G724	G659	G592	U527	U457	G394	U328	G266	G140
U1001	A1067	U	G941	G869	G802	G725	A660	C593	U528		U395	A329	G267	C141
G1002	U1002	G	U942	U870	C803	G727	U662	C594	G529	C461	U396		U268	A144
U1003	A943	U	U943	G871	G804	G728	U663	C595	G530	A462	U398	G332	U270	A145
C1004	U1004	C	U944	U872	G805		U664	C596	G531	A463	G333	G330	C271	U146
A1005	U1005	A	U945	U873	G806	U731	A665	C597	G532		C400	G334	A272	G147
C946	C946	C	C946	U874	A807	U732	A666	C598	A531	A466	U401	U335	G273	A148
U1007	U1007	U	U947	A875	A808	U733	C667	C599	U533	G467	U402	G336	G274	G149
C1008	G948	C	G948	A876	G809	U734	C668	G601	C534	U470	C403	A337	G275	G150
U1009	U949	U	U949	A877	G810	U735	C669	A602	G535		G404	C338		A151
G1010	G950	G	G950	G878	C811	U736	U670	A603	A536	A473	G406	C342	C279	A152
A1011	C1011	A	A951	C879	A812	U737	A671	G604	G537	C474	A407	C343	C280	C153
C952	G952	C	G952	C880	C813	U738	G672	C605	G538	G475	U409	C344	C281	C154
G953	G953	G	G953	A882	G814	G744	U675	U611	G539	A476	A410	G345	C282	C155
U1013	A1013	U	U954	U883	U815	G745	C676	U612	A540	A477	A411	U346	U283	G157
C1014	C1014	C	U955	U884	G816	G746	U677	C613	C541		C347	C348	C284	A158
U1015	G956	U	U956	G885	G817	U747	G681	U614	A542	C478	G412		A285	G159
C1016	A957	C	A957	U886	A818	U748	A682	G615	G543	C480	G413		U286	A160
U1017	G958	U	G958	U888	G820	U749	G683	U616	G544	U481	C414	A352	C287	A161
A1018	C959	A	C959	C889	G821	U750	G684	C617	G545	G482	A415	G353	U224	C162
C1019	G960	C	G960	C890	U822	U751	U685	G618	C546	C483	G416	A354	G225	U163
A1020	A961	A	A961	G891	C823	U752	A686	U619	A549	A484	A417		A226	G164
G1021	C962	G	C962	G892	U824	U753	U687	A620	C550	G487	C418	A357	C291	A165
C1022	G964	C	G964	C893	G825	U754	A688	C621	A551	U488	A419	G358	C292	A166
G1025	A965	G	A965	C896	U826	G755	G691	G622	A552	U489	U420	C361	C293	A167
U1026	U966	U	U966	A897	A827		A692	U623	A553	C490	G422	G362	C294	C168
G1027	U967	G	U967	G898	G830	U758	A693	U624	A554	G497	G428	G367	C295	A169
U1028	G968	U	G968	U902	U831	C759	A694	U625	A555	C491	A429	A302	U300	G175
C1029	G969	C	G969	G902	U832	U760	C695	U626	C556	U493	A423	A303	C239	U176
U1030	U970	U	U970	U903	G834	U761	C696	G627	C557		G424	C303	A241	A177
G1031	G	G	G	U904	U835	G765	C697	A628	C558	G496	U425	G304	A242	U178
A1032	U	U	U	C905	U836	G766	A698	A629	C559	A497	G426	G305	A243	G179
C1033	G	C	G	C906	U840	A767	C699	A630	A562	A498	C427	C301	C244	G180
G1034	U	U	U	A907	A841	G771	U700	A631	C563	G499	A430	G368	C245	G181
U1039	C	C	C	A908	C842		U701	C633	C564	G501	G431	G369	G246	G182
G1038	G	G	G	A843	A843	G772	G702	G634	A565	G502	G432	G370	U306	G183
A1040	C	C	C	A912	A844	U776	G703	A635	A566	U502	C433	U371	C246	G184
U1041	C	C	C	U845	U845	U777	G704	G636	U567	G503	U434	A372	G307	G185
U1042	U	U	U	A916	A846	C778	C705	C637	G574	G504		G375	A247	A183
C1043	C	C	C	U917	C847	U779	G706	C638	A575	G506	A437	C377	U310	G184
G1044	C	C	C	C848	C848		G707	A639	G576	A507		C378	A248	G186
U1045	G	G	G	C920	C849	C783	A708	G640	G577	A508	C440	A379	G249	A187
A	A	A	A	G921	U850	U785	G709	G641	G578	A509	A441	G379	C311	A188
G	G	G	G	A922	C851	U786	G710	G642	G579	U510	A442	A380	C250	G189
A923	U852	A	A923	G924	C852	U787	G711	A643	G580	A511	C443	G381	C251	C188
G924	C853	G	G924	U925	C854	A788	G712	A644	G581	A512	C444	U382	G252	U253
G	G	G	G	C925	G854	C789	U713	U645	G582	G512	U445	A383	G315	A191

C	U1996	A2060	U1996	G1932	A1865	C1792	G1730	A1661	U1599	U1539	U1473	G1398	G1332	G1263	C1196
U	A1997	C2061	A1997	G1933	A1866	C1793	G1731	C1662	G1600	G1540	C1474	A1399	U1333	U1264	G1197
A	G1998	U2062	G1998	C1934	G1867	G1794	C1732	G1663	G1601	G1541	C1475	G1401	C1334	U1265	U1198
G	C1999	U2063	C1999	C1935	G1868	G1795	A1732	A1664	C1602	G1542	A1476	G1401	C1335	U1266	A1199
C	G2000	U2064	G2000	C1936	U1871	A1796	C1733	G1665	G1603	G1543	C1477	U1407	U1336	C1267	A1200
G	C2001	C2065	G2001	U1937	G1872	G1798	A1734	G1666	G1604	U1544	U1478	U1408	G1337	C1268	C1201
G	C2002	C2066	C2002	G1938	C1873	C1799	C1735	A1667	G1605	C1545	G1479	U1409	U1338	C1269	A1202
G	U2003	A2067	U2003	U1939	G1873	G1799	C1736	U1668	A1606	G1546	A1480	G1409	U1339	U1270	A1203
C	U2004	C2068	U2004	C1940	U1874	G1800	A1737	G1669	A1607	A1547	G1481	U1412	C1342	U1271	C1204
C	G2005	U2069	G2005	A1941	A1875	A1801	C1738	A1670	G1608	U1548	A1482	U1412	C1343	G1272	U1205
A	C2006	G2070	C2006	A1942	A1876	G1802	G1739	A1671	G1609	C1549	A1483	G1344	C1344	G1273	U1206
C	U2007	C2071	A2007	G1943	U1878	C1803	U1740	G1672	G1610	A1550	G1484	U1419	A1345	A1274	A1207
C	G2008	G2072	U2008	G1944	U1879	A1804	U1741	U1673	G1611	C1551	G1485	C1420	U1346	C1275	C1208
C	G2009	C2073	G2009	G1945	U1880	G1805	A1742	C1674	A1612	G1552	A1486	C1421	U1347	C1209	C1209
A	A2010	A2074	A2010	G1946	U1883	G1806	G1743	C1675	G1613	C1553	A1487	U1422	U1350	A1278	G1210
G	C2011	G2075	A2011	G1947	G1884	U1814	C1750	C1676	G1614	C1554	A1488	C1423	G1351	U1279	G1211
A	G2012	U2076	U2012	G1948	A1886	G1815	G1752	A1677	A1615	G1555	A1489	A1424	A1352	A1280	C1212
C	G2013	C2013	G2013	G1949	A1887	C1810	G1753	A1678	A1616	G1556	U1492	C1426	G1353	C1281	C1213
A	G2014	A2081	G2014	G1950	U1887	U1748	A1754	C1679	G1617	G1557	A1493	C1427	G1354	U1282	G1214
A	A2015	C2082	A2015	G1951	C1888	U1749	A1755	C1680	G1618	C1558	A1494	C1428	G1357	A1287	A1215
C	A2083	A2083	A2016	U1889	C1889	C1750	G1756	G1681	G1619	A1559	A1495	U1432	A1357	G1288	G1216
A	U2017	C2087	U2017	A1890	A1815	G1751	G1752	A1682	G1620	U1561	C1496	U1433	U1357	G1289	U1218
G	A2018	G2088	A2018	G1891	C1818	C1819	A1753	A1684	G1622	G1562	G1497	A1434	U1359	G1292	A1222
G	A2019	C2089	G2019	G1894	G1820	A1755	A1755	C1685	G1623	C1563	G1498	U1435	G1360	U1293	G1223
A	A2022	G2093	A2022	U1899	G1828	G1756	A1756	C1687	A1625	C1565	U1500	U1436	G1361	U1294	G1224
A	G2023	G2094	G2023	C1898	A1829	G1757	U1758	A1688	A1626	C1566	A1501	A1437	U1362	A1295	A1225
A	C2025	U2095	C2025	A1900	C1830	U1758	A1759	A1689	G1627	G1567	A1502	G1438	G1363	A1296	
A	C2026	A2096	C2026	G1901	U1831	C1830	A1759	C1690	G1628	G1568	U1503	G1439	G1364	A1297	
C	U2027	C2097	U2027	C1902	U1831	G1760	G1760	A1691	G1629	U1569	A1504	U1440	G1365	C1228	C1228
U	C2028	C2098	C2028	U1903	A1904	U1761	C1761	C1692	A1630	C1570	U1505	U1441	G1366	C1229	C1229
A	U2029	C2099	U2029	A1904	C1834	U1762	C1762	A1693	A1631	G1571	U1506	A1442	A1369	G1230	A1230
C	A2030	A2099	A2030	U1905	U1835	C1763	C1763	G1697	G1632	A1572	C1507	G1443	G1370	U1234	U1234
C	C2031	G2100	C2031	C1906	U1835	G1764	G1765	U1698	G1633	A1573	G1444	G1445	U1371	C1302	U1235
A	U2032	A2101	U2032	U1907	U1838	G1766	A1767	C1768	G1634	C1574	G1445	U1446	A1372	A1236	A1236
A	G2033	G2102	G2033	G1908	A1839	A1840	U1766	U1702	U1635	C1575	U1511	U1447	G1373	U1237	U1237
C	U2034	C2104	C2034	A1909	A1841	A1842	A1767	A1702	G1636	G1576	C1512	A1448	A1375	C1238	C1238
C	C2035	C2105	C2035	A1910	U1842	A1842	C1768	U1702	A1637	U1577	C1513	U1449	G1376	G1239	G1239
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G	C2040	G2111	C2040	G1914	U1848	G1849	G1772	G1709	A1642	A1582	U1517	G1452	G1311	C1243	C1243
A	G2041	G2112	G2041	U1915	C1854	C1854	A1778	G1710	C1643	C1582	U1518	U1453	G1312	U1244	U1244
C	U2042	C2113	C2042	C1916	U1854	U1854	A1779	A1717	U1644	U1583	U1519	U1454	A1383	C1245	C1245
C	G2043	A2114	G2043	G1917	C1855	G1855	G1780	G1717	G1648	G1588	U1524	A1458	G1387	U1249	U1249
A	C2044	U2115	C2044	U1918	C1856	G1856	G1781	G1718	G1649	G1589	U1525	U1461	U1388	G1250	G1250
G	U2045	C2116	U2045	A1919	C1857	U1857	A1782	G1719	C1650	A1590	A1526	C1462	U1389	G1251	A1252
U	G2046	U2117	G2046	G1920	U1858	U1858	G1783	G1720	U1654	A1591	A1527	U1463	G1390	C1253	C1253
C	A2047	C2118	A2047	A1921	A1859	U1859	U1784	C1721	G1655	G1592	A1528	C1464	G1391	C1254	C1254
A	C2048	U2119	C2048	G1922	U1860	U1860	G1785	G1722	A1656	C1593	U1531	G1468	A1392	G1255	A1255
C	G2049	C2120	G2049	A1923	U1861	U1861	G1786	G1723	G1656	C1594	U1532	C1469	A1393	G1256	
G	U2050	U2121	U2050	G1924	C1862	U1862	U1787	G1724	A1657	G1595	U1533	C1470	C1394	G1257	A1259
U	C2051	C2122	C2051	A1925	G1863	U1863	G1788	U1725	A1658	U1596	G1535	A1471	C1395	C1258	G1260
A	U2052	G2123	U2052	G1926	G1864	U1864	U1789	G1726	A1659	A1597	U1536	C1472	C1397	A1261	C1262
C	G2053	C2243	G2053	A1927	C1865	U1865	G1790	G1727	G1660	U1598	C1538				
C	A2054	U2244	A2054	U1928	C1866	U1866	U1791	G1727							
C	C2055	G2245	C2055	C1929	G1867	U1867	U1792	G1728							
C	U2056	C2246	U2056	A1930	G1868	U1868	U1793	G1729							
C	U2057	C2247	U2057	G1931	G1869	U1869	U1794	G1730							
G	C2248	C2248	C2248	G1932	G1870	U1870	U1795	G1731							



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.01Å 299.25Å 573.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 85.53 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 89.1 (85.53-2.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.226 0.187 , 0.260	Depositor DCC
R_{free} test set	2448 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 95.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 667044 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/1786	0.66	0/2408
2	B	0.38	0/2690	0.67	0/3652
3	C	0.42	0/1885	0.65	0/2552
4	D	0.35	0/1111	0.58	0/1498
5	E	0.36	0/1382	0.61	0/1880
6	F	0.36	0/901	0.60	0/1224
7	G	0.40	0/241	0.53	0/324
8	H	0.36	0/1302	0.66	0/1743
9	I	0.33	0/526	0.54	0/716
10	J	0.42	0/1136	0.63	0/1530
11	K	0.40	0/1004	0.71	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.41	0/1582	0.64	0/2116
14	N	0.33	0/1474	0.62	0/1999
15	O	0.37	0/874	0.64	0/1181
16	P	0.39	0/1147	0.56	0/1528
17	Q	0.37	0/749	0.67	0/1005
18	R	1.28	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.38	0/648	0.59	0/875
20	T	0.39	0/958	0.67	0/1289
21	U	0.46	0/417	0.64	0/562
22	V	0.35	0/502	0.56	0/675
23	W	0.41	0/1219	0.68	0/1655
24	X	0.39	0/664	0.62	0/895
25	Y	0.39	0/1146	0.64	0/1536
26	Z	0.42	0/584	0.63	0/781
27	1	0.47	0/438	0.63	0/578
28	2	0.38	0/401	0.61	0/529
29	3	0.43	0/771	0.67	0/1024
30	0	0.49	0/65957	0.70	6/102867 (0.0%)
31	9	0.37	0/2904	0.68	0/4526
All	All	0.48	7/98701 (0.0%)	0.69	12/147586 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
23	W	0	1
30	0	0	19
All	All	1	20

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.13	2.85	1.50
18	R	150	PRO	CA-C	-18.46	1.16	1.52
18	R	150	PRO	CG-CD	14.04	1.97	1.50
18	R	150	PRO	C-O	11.94	1.47	1.23
18	R	150	PRO	N-CA	11.49	1.66	1.47

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.46	55.84	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.12	128.68	111.70
18	R	150	PRO	N-CA-CB	11.03	116.54	103.30
18	R	150	PRO	CA-C-O	-8.33	100.20	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	493	U	Sidechain
30	0	788	A	Sidechain
30	0	862	U	Sidechain
30	0	882	A	Sidechain
23	W	90	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	123	0
2	B	2625	0	2533	168	0
3	C	1860	0	1813	98	0
4	D	1094	0	1085	71	0
5	E	1357	0	1266	49	0
6	F	890	0	843	39	0
7	G	240	0	231	18	0
8	H	1282	0	1292	62	0
9	I	519	0	500	24	0
10	J	1120	0	1098	56	0
11	K	994	0	1027	54	0
12	L	1118	0	1076	54	0
13	M	1558	0	1573	120	0
14	N	1445	0	1401	74	0
15	O	865	0	873	47	0
16	P	1136	0	1123	64	0
17	Q	735	0	729	32	0
18	R	1149	0	1122	58	0
19	S	641	0	605	29	0
20	T	950	0	924	56	0
21	U	410	0	368	58	0
22	V	499	0	511	26	0
23	W	1196	0	1137	79	0
24	X	654	0	653	42	0
25	Y	1130	0	1133	69	0
26	Z	573	0	534	84	0
27	1	431	0	426	27	0
28	2	396	0	413	20	0
29	3	755	0	732	138	0
30	0	59020	0	29802	3476	0
31	9	2599	0	1325	195	0
32	0	85	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	T	1	0	0	0	0
32	Y	2	0	0	0	0
33	0	1	0	0	0	0
33	M	1	0	0	0	0
34	0	63	0	0	0	0
34	9	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	3	0	0	0	0
34	S	1	0	0	0	0
35	0	8	0	0	6	0
35	3	1	0	0	4	0
35	A	1	0	0	0	0
35	B	1	0	0	1	0
35	J	4	0	0	4	0
35	L	1	0	0	0	0
35	M	1	0	0	2	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	Q	1	0	0	1	0
35	R	1	0	0	0	0
35	Y	1	0	0	1	0
36	0	93	0	0	0	0
36	1	2	0	0	0	0
36	2	1	0	0	0	0
36	3	2	0	0	0	0
36	9	2	0	0	0	0
36	A	2	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	J	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	0	5813	0	0	458	0
38	1	53	0	0	3	0
38	2	48	0	0	0	0
38	3	80	0	0	12	0
38	9	144	0	0	18	0
38	A	122	0	0	13	0
38	B	158	0	0	21	0
38	C	176	0	0	16	0
38	D	51	0	0	7	0
38	E	51	0	0	3	0
38	F	27	0	0	2	0
38	G	15	0	0	1	0
38	H	73	0	0	2	0
38	I	3	0	0	0	0
38	J	55	0	0	4	0
38	K	61	0	0	5	0
38	L	99	0	0	11	0
38	M	148	0	0	15	0
38	N	56	0	0	7	0
38	O	42	0	0	3	0
38	P	56	0	0	4	0
38	Q	58	0	0	5	0
38	R	78	0	0	1	0
38	S	37	0	0	3	0
38	T	41	0	0	3	0
38	U	34	0	0	4	0
38	V	10	0	0	2	0
38	W	71	0	0	4	0
38	X	28	0	0	1	0
38	Y	102	0	0	8	0
38	Z	33	0	0	7	0
All	All	99122	0	59914	5051	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 5051 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CD	18:R:150:PRO:CG	1.97	1.43
30:0:871:G:C8	30:0:871:G:H5'	1.74	1.22
31:9:29:C:H2'	31:9:30:C:H5'	1.21	1.17
14:N:37:ARG:NH1	31:9:6:C:H5''	1.59	1.16

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:56:A:H2'	31:9:57:A:H5''	1.23	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	198 (84%)	28 (12%)	9 (4%)	5	10
2	B	335/338 (99%)	287 (86%)	42 (12%)	6 (2%)	13	31
3	C	244/246 (99%)	211 (86%)	29 (12%)	4 (2%)	14	35
4	D	134/177 (76%)	109 (81%)	22 (16%)	3 (2%)	10	25
5	E	170/178 (96%)	152 (89%)	16 (9%)	2 (1%)	19	45
6	F	117/120 (98%)	102 (87%)	11 (9%)	4 (3%)	6	12
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	12	29
9	I	68/162 (42%)	56 (82%)	10 (15%)	2 (3%)	7	16
10	J	140/145 (97%)	125 (89%)	12 (9%)	3 (2%)	11	27
11	K	130/132 (98%)	107 (82%)	21 (16%)	2 (2%)	15	38
12	L	141/165 (86%)	112 (79%)	25 (18%)	4 (3%)	8	18
13	M	192/196 (98%)	165 (86%)	22 (12%)	5 (3%)	8	20
14	N	184/187 (98%)	156 (85%)	23 (12%)	5 (3%)	8	19
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	125 (89%)	13 (9%)	3 (2%)	11	27
17	Q	93/96 (97%)	82 (88%)	7 (8%)	4 (4%)	4	8
18	R	148/155 (96%)	132 (89%)	15 (10%)	1 (1%)	30	62
19	S	79/85 (93%)	67 (85%)	11 (14%)	1 (1%)	18	43
20	T	117/120 (98%)	95 (81%)	18 (15%)	4 (3%)	6	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	51/67 (76%)	46 (90%)	3 (6%)	2 (4%)	5	10
22	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	14	35
23	W	152/154 (99%)	129 (85%)	21 (14%)	2 (1%)	18	43
24	X	80/92 (87%)	68 (85%)	8 (10%)	4 (5%)	3	6
25	Y	140/241 (58%)	131 (94%)	8 (6%)	1 (1%)	30	62
26	Z	71/116 (61%)	52 (73%)	13 (18%)	6 (8%)	1	1
27	1	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	12	29
28	2	42/50 (84%)	37 (88%)	4 (10%)	1 (2%)	9	22
29	3	90/92 (98%)	73 (81%)	14 (16%)	3 (3%)	6	13
All	All	3705/4472 (83%)	3193 (86%)	426 (12%)	86 (2%)	10	24

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLY
4	D	65	GLU
4	D	137	PRO
6	F	61	MET
6	F	101	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	172 (96%)	7 (4%)	43	76
2	B	282/283 (100%)	261 (93%)	21 (7%)	20	43
3	C	193/193 (100%)	178 (92%)	15 (8%)	18	40
4	D	117/148 (79%)	109 (93%)	8 (7%)	22	48
5	E	152/156 (97%)	146 (96%)	6 (4%)	43	76
6	F	93/94 (99%)	89 (96%)	4 (4%)	40	72
7	G	27/282 (10%)	25 (93%)	2 (7%)	20	43
8	H	134/145 (92%)	125 (93%)	9 (7%)	23	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	58/130 (45%)	55 (95%)	3 (5%)	32	63
10	J	118/121 (98%)	112 (95%)	6 (5%)	33	64
11	K	106/106 (100%)	98 (92%)	8 (8%)	19	43
12	L	113/127 (89%)	105 (93%)	8 (7%)	21	46
13	M	158/160 (99%)	148 (94%)	10 (6%)	25	53
14	N	149/150 (99%)	143 (96%)	6 (4%)	42	75
15	O	93/94 (99%)	90 (97%)	3 (3%)	51	82
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	93
17	Q	79/80 (99%)	75 (95%)	4 (5%)	33	64
18	R	117/122 (96%)	110 (94%)	7 (6%)	27	56
19	S	71/74 (96%)	67 (94%)	4 (6%)	30	59
20	T	105/106 (99%)	97 (92%)	8 (8%)	19	41
21	U	44/53 (83%)	42 (96%)	2 (4%)	38	70
22	V	51/57 (90%)	48 (94%)	3 (6%)	28	56
23	W	130/130 (100%)	124 (95%)	6 (5%)	37	70
24	X	66/74 (89%)	57 (86%)	9 (14%)	5	13
25	Y	120/196 (61%)	115 (96%)	5 (4%)	40	73
26	Z	60/94 (64%)	54 (90%)	6 (10%)	11	25
27	1	46/47 (98%)	45 (98%)	1 (2%)	64	90
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	89
29	3	79/79 (100%)	75 (95%)	4 (5%)	33	64
All	All	3095/3646 (85%)	2917 (94%)	178 (6%)	28	57

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	132	LEU
13	M	76	ARG
25	Y	220	GLU
11	K	12	LEU
12	L	18	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	58	GLN
14	N	107	ASN
28	2	36	ASN
13	M	24	GLN
13	M	170	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	263 (9%)	14 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	281 (9%)	15 (0%)

5 of 281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	11	A
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1237	U
30	0	1352	A
30	0	2526	C
30	0	871	G
30	0	2466	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	0	2587	30	20,22,23	0.64	0	24,31,34	0.68	0
30	OMG	0	2588	30	24,26,27	0.82	1 (4%)	32,38,41	5.09	3 (9%)
30	UR3	0	2619	30	20,22,23	0.88	1 (5%)	23,32,35	0.82	0
30	PSU	0	2621	30	19,21,22	1.20	3 (15%)	23,30,33	1.04	1 (4%)
30	1MA	0	628	30,34	23,25,26	0.80	0	32,37,40	1.01	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/10/27/28	0/1/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30,34	-	0/8/25/26	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	2.67	1.42	1.37
30	0	2621	PSU	C6-N1	2.49	1.34	1.32
30	0	2619	UR3	P-OP1	2.39	1.49	1.46
30	0	2621	PSU	P-OP1	2.12	1.49	1.46
30	0	2588	OMG	P-OP1	2.07	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.18	130.34	134.14
30	0	2588	OMG	C6-N1-C2	3.25	125.19	119.51
30	0	628	1MA	C2-N3-C4	-3.17	110.82	116.23
30	0	2588	OMG	C2-N3-C4	-2.30	111.86	115.09
30	0	2621	PSU	C5-C4-N3	-2.21	114.84	118.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	0.52	31 (13%) 4 4	36, 78, 117, 135	0
2	B	337/338 (99%)	0.24	23 (6%) 17 19	36, 72, 106, 116	0
3	C	246/246 (100%)	0.11	14 (5%) 23 25	31, 60, 87, 97	0
4	D	140/177 (79%)	2.24	63 (45%) 1 0	91, 126, 152, 162	0
5	E	172/178 (96%)	0.38	13 (7%) 14 14	62, 89, 116, 123	0
6	F	119/120 (99%)	1.10	29 (24%) 1 1	68, 96, 130, 142	0
7	G	29/348 (8%)	1.66	12 (41%) 1 0	104, 117, 126, 127	0
8	H	160/177 (90%)	0.98	33 (20%) 1 2	57, 81, 125, 130	0
9	I	70/162 (43%)	3.30	44 (62%) 0 0	149, 172, 188, 190	0
10	J	142/145 (97%)	0.46	15 (10%) 7 7	48, 67, 90, 114	0
11	K	132/132 (100%)	0.12	5 (3%) 38 43	38, 69, 98, 107	0
12	L	145/165 (87%)	1.29	40 (27%) 1 1	50, 96, 141, 147	0
13	M	194/196 (98%)	0.99	30 (15%) 3 3	41, 61, 109, 119	0
14	N	186/187 (99%)	1.36	59 (31%) 1 1	72, 94, 145, 152	0
15	O	115/116 (99%)	0.42	13 (11%) 6 6	57, 72, 93, 98	0
16	P	143/149 (95%)	0.38	13 (9%) 9 9	52, 74, 92, 103	0
17	Q	95/96 (98%)	0.91	18 (18%) 2 2	55, 71, 88, 103	0
18	R	150/155 (96%)	0.11	8 (5%) 25 28	45, 61, 87, 109	0
19	S	81/85 (95%)	0.56	11 (13%) 4 4	61, 80, 103, 113	0
20	T	119/120 (99%)	0.86	21 (17%) 2 2	51, 74, 105, 132	0
21	U	53/67 (79%)	6.49	51 (96%) 0 0	119, 128, 137, 138	0
22	V	65/71 (91%)	1.50	23 (35%) 1 1	68, 97, 141, 146	0
23	W	154/154 (100%)	0.82	28 (18%) 2 2	49, 66, 88, 103	0
24	X	82/92 (89%)	1.22	20 (24%) 1 1	57, 81, 104, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.12	6 (4%) 35 39	39, 59, 87, 116	0
26	Z	73/116 (62%)	9.76	63 (86%) 0 0	109, 128, 137, 141	0
27	1	56/57 (98%)	0.11	1 (1%) 65 71	34, 47, 56, 60	0
28	2	46/50 (92%)	1.00	13 (28%) 1 1	43, 84, 116, 122	0
29	3	92/92 (100%)	9.09	90 (97%) 0 0	112, 132, 141, 144	0
30	0	2754/2923 (94%)	-0.37	14 (0%) 88 92	31, 64, 118, 195	0
31	9	122/122 (100%)	-0.54	1 (0%) 83 87	53, 94, 121, 167	0
All	All	6651/7517 (88%)	0.52	805 (12%) 5 5	31, 72, 133, 195	0

The worst 5 of 805 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	41	GLU	30.8
26	Z	45	VAL	30.4
26	Z	35	SER	30.0
29	3	45	GLY	29.2
26	Z	50	VAL	28.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	OMU	0	2587	21/22	0.12	0.10	51,52,54,56	0
30	1MA	0	628	23/24	0.15	-0.51	37,44,45,46	0
30	PSU	0	2621	20/21	0.17	-0.63	49,51,60,60	0
30	UR3	0	2619	21/22	0.14	-0.86	56,57,60,60	0
30	OMG	0	2588	24/25	0.14	-1.01	48,51,54,55	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	K	0	8401	1/1	0.60	93.40	145,145,145,145	0
36	SR	0	9007	1/1	1.13	75.13	200,200,200,200	0
34	NA	0	8574	1/1	1.40	75.07	92,92,92,92	0
36	SR	0	8982	1/1	0.89	68.93	200,200,200,200	0
34	NA	0	8562	1/1	1.25	56.62	83,83,83,83	0
35	CL	0	8822	1/1	0.89	51.63	140,140,140,140	0
34	NA	0	8559	1/1	0.68	46.00	96,96,96,96	0
32	MG	0	8037	1/1	0.33	42.11	92,92,92,92	0
35	CL	B	8819	1/1	1.21	42.07	83,83,83,83	0
36	SR	0	8974	1/1	0.45	36.15	196,196,196,196	0
34	NA	0	8525	1/1	0.54	35.67	113,113,113,113	0
34	NA	0	8547	1/1	0.49	34.80	115,115,115,115	0
36	SR	0	8957	1/1	1.43	32.80	200,200,200,200	0
36	SR	0	8979	1/1	0.44	31.31	200,200,200,200	0
34	NA	0	8544	1/1	0.56	30.85	76,76,76,76	0
34	NA	0	8554	1/1	0.76	27.23	124,124,124,124	0
34	NA	0	8545	1/1	0.55	25.81	74,74,74,74	0
34	NA	0	8518	1/1	0.79	24.10	91,91,91,91	0
36	SR	0	9004	1/1	1.39	23.34	200,200,200,200	0
32	MG	0	8030	1/1	0.92	23.00	75,75,75,75	0
34	NA	0	8536	1/1	0.18	22.75	64,64,64,64	0
32	MG	0	8049	1/1	0.37	22.33	82,82,82,82	0
36	SR	0	8964	1/1	0.27	19.68	176,176,176,176	0
35	CL	0	8815	1/1	0.41	19.48	130,130,130,130	0
35	CL	J	8816	1/1	2.00	18.71	99,99,99,99	0
34	NA	0	8571	1/1	0.36	18.64	99,99,99,99	0
32	MG	0	8089	1/1	0.36	17.94	56,56,56,56	0
34	NA	0	8524	1/1	0.54	17.35	53,53,53,53	0
34	NA	0	8558	1/1	0.39	16.88	82,82,82,82	0
34	NA	0	8509	1/1	0.43	15.94	84,84,84,84	0
36	SR	0	8922	1/1	0.28	14.56	181,181,181,181	0
34	NA	R	8575	1/1	0.40	14.27	97,97,97,97	0
34	NA	B	8552	1/1	0.59	13.97	70,70,70,70	0
32	MG	0	8047	1/1	0.69	13.94	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8998	1/1	0.52	12.72	200,200,200,200	0
36	SR	0	8996	1/1	0.39	12.22	200,200,200,200	0
34	NA	0	8549	1/1	0.25	12.17	96,96,96,96	0
32	MG	0	8078	1/1	0.49	12.03	72,72,72,72	0
32	MG	0	8081	1/1	0.29	11.85	116,116,116,116	0
36	SR	0	8969	1/1	1.81	11.25	200,200,200,200	0
34	NA	0	8564	1/1	0.28	10.73	87,87,87,87	0
36	SR	0	8926	1/1	0.25	10.64	131,131,131,131	0
34	NA	0	8567	1/1	0.44	10.53	83,83,83,83	0
32	MG	0	8066	1/1	0.30	10.19	71,71,71,71	0
34	NA	0	8563	1/1	0.44	9.94	66,66,66,66	0
32	MG	Y	8077	1/1	0.34	9.89	58,58,58,58	0
35	CL	0	8805	1/1	0.31	9.73	105,105,105,105	0
32	MG	0	8079	1/1	0.28	9.37	57,57,57,57	0
34	NA	0	8522	1/1	0.33	9.34	130,130,130,130	0
34	NA	L	8568	1/1	0.50	9.02	59,59,59,59	0
34	NA	0	8542	1/1	0.38	9.02	79,79,79,79	0
34	NA	0	8528	1/1	0.37	8.87	113,113,113,113	0
32	MG	0	8039	1/1	0.44	8.83	94,94,94,94	0
36	SR	0	8924	1/1	0.21	8.49	131,131,131,131	0
36	SR	0	8971	1/1	0.21	8.46	200,200,200,200	0
36	SR	0	8905	1/1	0.28	7.83	68,68,68,68	0
34	NA	0	8546	1/1	0.79	7.81	108,108,108,108	0
36	SR	0	8941	1/1	0.23	7.50	141,141,141,141	0
34	NA	0	8506	1/1	0.30	7.34	91,91,91,91	0
34	NA	0	8566	1/1	0.35	7.03	86,86,86,86	0
34	NA	0	8561	1/1	0.28	6.93	53,53,53,53	0
32	MG	0	8048	1/1	0.31	6.81	26,26,26,26	0
32	MG	0	8008	1/1	0.20	6.34	26,26,26,26	0
34	NA	0	8527	1/1	0.36	5.97	92,92,92,92	0
34	NA	0	8501	1/1	0.23	5.87	53,53,53,53	0
36	SR	0	8925	1/1	0.16	5.73	98,98,98,98	0
36	SR	B	8987	1/1	0.78	5.63	200,200,200,200	0
34	NA	0	8516	1/1	0.21	5.60	27,27,27,27	0
36	SR	0	8951	1/1	0.18	5.52	183,183,183,183	0
32	MG	0	8023	1/1	0.20	5.52	38,38,38,38	0
34	NA	0	8517	1/1	0.21	5.43	69,69,69,69	0
36	SR	0	8946	1/1	0.26	5.31	144,144,144,144	0
32	MG	0	8033	1/1	0.16	5.26	69,69,69,69	0
36	SR	0	8994	1/1	0.36	5.20	200,200,200,200	0
36	SR	0	8903	1/1	0.22	5.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	CL	0	8813	1/1	0.20	5.11	64,64,64,64	0
34	NA	0	8514	1/1	0.39	5.10	74,74,74,74	0
34	NA	0	8553	1/1	0.27	5.04	81,81,81,81	0
34	NA	0	8502	1/1	0.26	5.00	66,66,66,66	0
34	NA	0	8508	1/1	0.21	4.93	118,118,118,118	0
32	MG	0	8036	1/1	0.15	4.87	62,62,62,62	0
34	NA	0	8534	1/1	0.39	4.82	53,53,53,53	0
32	MG	0	8070	1/1	0.17	4.75	39,39,39,39	0
35	CL	O	8808	1/1	0.69	4.62	114,114,114,114	0
36	SR	9	8980	1/1	0.17	4.48	191,191,191,191	0
35	CL	N	8807	1/1	0.60	4.38	99,99,99,99	0
32	MG	0	8022	1/1	0.18	4.32	25,25,25,25	0
32	MG	9	8074	1/1	0.21	4.29	97,97,97,97	0
32	MG	9	8040	1/1	0.20	4.10	101,101,101,101	0
35	CL	A	8809	1/1	0.37	4.09	116,116,116,116	0
36	SR	R	8912	1/1	0.24	3.89	107,107,107,107	0
36	SR	0	8983	1/1	0.25	3.80	200,200,200,200	0
32	MG	0	8009	1/1	0.23	3.79	24,24,24,24	0
34	NA	0	8537	1/1	0.26	3.75	46,46,46,46	0
34	NA	0	8551	1/1	0.22	3.68	75,75,75,75	0
36	SR	0	9000	1/1	0.19	3.58	200,200,200,200	0
32	MG	0	8043	1/1	0.22	3.52	62,62,62,62	0
34	NA	0	8512	1/1	0.23	3.43	40,40,40,40	0
34	NA	0	8556	1/1	0.43	3.38	94,94,94,94	0
34	NA	0	8535	1/1	0.15	3.14	58,58,58,58	0
32	MG	0	8064	1/1	0.23	3.08	51,51,51,51	0
36	SR	0	8939	1/1	0.16	3.08	155,155,155,155	0
36	SR	0	8958	1/1	0.17	3.02	126,126,126,126	0
32	MG	0	8029	1/1	0.20	2.96	62,62,62,62	0
32	MG	0	8071	1/1	0.18	2.87	78,78,78,78	0
36	SR	0	8931	1/1	0.13	2.84	120,120,120,120	0
36	SR	J	8986	1/1	0.17	2.79	200,200,200,200	0
34	NA	0	8530	1/1	0.25	2.68	53,53,53,53	0
35	CL	Q	8811	1/1	0.40	2.55	124,124,124,124	0
34	NA	0	8531	1/1	0.16	2.48	54,54,54,54	0
34	NA	0	8555	1/1	0.23	2.27	80,80,80,80	0
34	NA	Q	8540	1/1	0.38	2.23	74,74,74,74	0
35	CL	J	8821	1/1	0.25	2.19	99,99,99,99	0
32	MG	0	8061	1/1	0.30	2.18	47,47,47,47	0
32	MG	0	8011	1/1	0.23	2.16	33,33,33,33	0
36	SR	0	8904	1/1	0.23	2.08	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8001	1/1	0.19	2.04	42,42,42,42	0
35	CL	M	8818	1/1	0.33	2.03	58,58,58,58	0
34	NA	0	8521	1/1	0.24	2.02	40,40,40,40	0
36	SR	0	8937	1/1	0.26	2.01	126,126,126,126	0
36	SR	0	8970	1/1	0.13	1.99	158,158,158,158	0
32	MG	0	8038	1/1	0.21	1.98	94,94,94,94	0
32	MG	0	8067	1/1	0.27	1.86	47,47,47,47	0
32	MG	0	8082	1/1	0.25	1.82	62,62,62,62	0
32	MG	0	8012	1/1	0.20	1.81	26,26,26,26	0
36	SR	0	8965	1/1	0.20	1.75	160,160,160,160	0
35	CL	0	8814	1/1	0.33	1.74	51,51,51,51	0
32	MG	0	8083	1/1	0.19	1.71	58,58,58,58	0
32	MG	0	8005	1/1	0.23	1.57	24,24,24,24	0
34	NA	0	8548	1/1	0.15	1.47	44,44,44,44	0
32	MG	0	8003	1/1	0.18	1.37	27,27,27,27	0
35	CL	J	8801	1/1	0.32	1.29	85,85,85,85	0
36	SR	0	8914	1/1	0.22	1.29	133,133,133,133	0
32	MG	0	8076	1/1	0.17	1.28	76,76,76,76	0
32	MG	0	8020	1/1	0.15	1.26	50,50,50,50	0
34	NA	0	8529	1/1	0.15	1.24	61,61,61,61	0
36	SR	0	8956	1/1	0.21	1.13	200,200,200,200	0
32	MG	0	8093	1/1	0.19	1.09	48,48,48,48	0
32	MG	A	8051	1/1	0.35	1.09	95,95,95,95	0
32	MG	0	8035	1/1	0.14	1.07	76,76,76,76	0
32	MG	0	8084	1/1	0.14	0.98	37,37,37,37	0
34	NA	0	8523	1/1	0.17	0.94	51,51,51,51	0
36	SR	0	8968	1/1	0.18	0.92	175,175,175,175	0
32	MG	Y	8086	1/1	0.19	0.80	52,52,52,52	0
36	SR	S	8961	1/1	0.12	0.79	130,130,130,130	0
34	NA	R	8532	1/1	0.18	0.77	68,68,68,68	0
32	MG	K	8054	1/1	0.15	0.75	42,42,42,42	0
36	SR	0	8935	1/1	0.14	0.73	101,101,101,101	0
36	SR	0	8907	1/1	0.15	0.73	60,60,60,60	0
36	SR	0	8915	1/1	0.14	0.63	123,123,123,123	0
36	SR	0	8963	1/1	0.14	0.60	117,117,117,117	0
34	NA	0	8504	1/1	0.17	0.58	41,41,41,41	0
34	NA	0	8560	1/1	0.67	0.52	80,80,80,80	0
34	NA	9	8543	1/1	0.24	0.48	51,51,51,51	0
36	SR	0	8985	1/1	0.12	0.37	168,168,168,168	0
32	MG	0	8088	1/1	0.15	0.31	53,53,53,53	0
36	SR	A	8929	1/1	0.20	0.25	139,139,139,139	0
36	SR	0	8906	1/1	0.16	0.21	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	F	9005	1/1	0.17	0.21	170,170,170,170	0
34	NA	0	8526	1/1	0.11	0.18	67,67,67,67	0
36	SR	0	8928	1/1	0.12	0.10	156,156,156,156	0
36	SR	0	8933	1/1	0.16	0.06	126,126,126,126	0
36	SR	0	9001	1/1	0.12	-0.01	200,200,200,200	0
34	NA	0	8513	1/1	0.18	-0.05	67,67,67,67	0
32	MG	0	8063	1/1	0.15	-0.09	60,60,60,60	0
34	NA	0	8557	1/1	0.10	-0.12	70,70,70,70	0
34	NA	0	8507	1/1	0.16	-0.18	38,38,38,38	0
33	K	M	8402	1/1	0.22	-0.22	96,96,96,96	0
35	CL	Y	8820	1/1	0.16	-0.23	58,58,58,58	0
34	NA	0	8541	1/1	0.18	-0.26	60,60,60,60	0
32	MG	0	8062	1/1	0.18	-0.27	66,66,66,66	0
32	MG	0	8002	1/1	0.15	-0.33	31,31,31,31	0
34	NA	9	8572	1/1	0.09	-0.35	71,71,71,71	0
35	CL	0	8803	1/1	0.13	-0.36	82,82,82,82	0
36	SR	0	8972	1/1	0.14	-0.39	138,138,138,138	0
35	CL	0	8817	1/1	0.14	-0.43	84,84,84,84	0
32	MG	0	8080	1/1	0.17	-0.45	65,65,65,65	0
36	SR	0	8901	1/1	0.14	-0.48	73,73,73,73	0
32	MG	0	8027	1/1	0.12	-0.51	44,44,44,44	0
32	MG	0	8015	1/1	0.13	-0.52	30,30,30,30	0
36	SR	0	8954	1/1	0.13	-0.52	115,115,115,115	0
36	SR	0	8976	1/1	0.17	-0.54	195,195,195,195	0
34	NA	0	8570	1/1	0.11	-0.55	57,57,57,57	0
34	NA	0	8573	1/1	0.17	-0.58	89,89,89,89	0
36	SR	0	9002	1/1	0.09	-0.62	200,200,200,200	0
32	MG	0	8026	1/1	0.10	-0.64	37,37,37,37	0
37	CD	Z	8703	1/1	0.48	-0.66	188,188,188,188	0
36	SR	0	8991	1/1	0.10	-0.67	188,188,188,188	0
34	NA	M	8539	1/1	0.14	-0.69	38,38,38,38	0
32	MG	0	8069	1/1	0.16	-0.70	73,73,73,73	0
32	MG	0	8090	1/1	0.10	-0.76	57,57,57,57	0
36	SR	3	8999	1/1	0.45	-0.76	200,200,200,200	0
32	MG	0	8053	1/1	0.10	-0.78	88,88,88,88	0
32	MG	0	8028	1/1	0.12	-0.81	13,13,13,13	0
32	MG	0	8041	1/1	0.15	-0.83	25,25,25,25	0
36	SR	A	8930	1/1	0.12	-0.85	131,131,131,131	0
34	NA	0	8569	1/1	0.15	-0.86	71,71,71,71	0
36	SR	0	8977	1/1	0.13	-0.86	200,200,200,200	0
34	NA	0	8519	1/1	0.16	-0.87	51,51,51,51	0
32	MG	0	8010	1/1	0.14	-0.90	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8992	1/1	0.11	-0.94	141,141,141,141	0
36	SR	0	8936	1/1	0.13	-0.96	114,114,114,114	0
32	MG	0	8019	1/1	0.16	-1.03	19,19,19,19	0
36	SR	0	8990	1/1	0.14	-1.07	113,113,113,113	0
36	SR	0	8943	1/1	0.11	-1.07	89,89,89,89	0
32	MG	T	8057	1/1	0.09	-1.08	80,80,80,80	0
34	NA	J	8538	1/1	0.14	-1.11	84,84,84,84	0
32	MG	0	8016	1/1	0.14	-1.15	41,41,41,41	0
34	NA	R	8533	1/1	0.10	-1.16	94,94,94,94	0
37	CD	U	8701	1/1	0.43	-1.16	180,180,180,180	0
36	SR	2	8947	1/1	0.14	-1.16	195,195,195,195	0
32	MG	0	8058	1/1	0.06	-1.17	7,7,7,7	0
32	MG	0	8056	1/1	0.14	-1.19	47,47,47,47	0
36	SR	0	8953	1/1	0.27	-1.20	179,179,179,179	0
37	CD	3	8704	1/1	0.62	-1.31	183,183,183,183	0
37	CD	1	8702	1/1	0.10	-1.32	78,78,78,78	0
35	CL	J	8802	1/1	0.12	-1.34	86,86,86,86	0
36	SR	3	8932	1/1	0.18	-1.35	148,148,148,148	0
34	NA	0	8515	1/1	0.11	-1.35	35,35,35,35	0
36	SR	0	8967	1/1	0.09	-1.37	163,163,163,163	0
34	NA	C	8503	1/1	0.11	-1.38	36,36,36,36	0
36	SR	0	8918	1/1	0.11	-1.46	88,88,88,88	0
36	SR	0	8981	1/1	0.12	-1.48	198,198,198,198	0
35	CL	L	8810	1/1	0.13	-1.50	91,91,91,91	0
32	MG	0	8052	1/1	0.11	-1.71	63,63,63,63	0
35	CL	0	8812	1/1	0.07	-1.75	70,70,70,70	0
34	NA	0	8565	1/1	0.08	-1.76	85,85,85,85	0
36	SR	0	8909	1/1	0.11	-1.83	100,100,100,100	0
32	MG	0	8085	1/1	0.10	-2.01	67,67,67,67	0
36	SR	0	8911	1/1	0.09	-2.05	100,100,100,100	0
36	SR	0	8993	1/1	0.06	-2.05	200,200,200,200	0
36	SR	0	8908	1/1	0.09	-2.06	99,99,99,99	0
34	NA	0	8505	1/1	0.14	-2.09	37,37,37,37	0
36	SR	0	8988	1/1	0.06	-2.14	200,200,200,200	0
36	SR	0	8959	1/1	0.06	-2.17	190,190,190,190	0
36	SR	0	8921	1/1	0.07	-2.22	88,88,88,88	0
32	MG	0	8065	1/1	0.11	-2.29	66,66,66,66	0
32	MG	0	8060	1/1	0.03	-2.30	58,58,58,58	0
32	MG	A	8050	1/1	0.08	-2.30	69,69,69,69	0
32	MG	0	8044	1/1	0.07	-2.34	59,59,59,59	0
36	SR	1	8952	1/1	0.13	-2.38	92,92,92,92	0
32	MG	0	8014	1/1	0.08	-2.45	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8938	1/1	0.05	-2.52	200,200,200,200	0
34	NA	0	8511	1/1	0.09	-2.59	53,53,53,53	0
36	SR	0	8960	1/1	0.06	-2.59	156,156,156,156	0
35	CL	R	8806	1/1	0.14	-2.60	66,66,66,66	0
36	SR	0	8948	1/1	0.09	-2.65	110,110,110,110	0
32	MG	0	8055	1/1	0.09	-2.67	60,60,60,60	0
35	CL	3	8804	1/1	0.08	-2.75	98,98,98,98	0
32	MG	0	8034	1/1	0.06	-2.84	50,50,50,50	0
36	SR	0	8984	1/1	0.05	-2.86	124,124,124,124	0
36	SR	0	8975	1/1	0.06	-2.89	189,189,189,189	0
36	SR	0	8940	1/1	0.07	-2.99	93,93,93,93	0
36	SR	9	9003	1/1	0.05	-3.00	200,200,200,200	0
36	SR	0	8944	1/1	0.08	-3.01	168,168,168,168	0
34	NA	S	8510	1/1	0.04	-3.06	41,41,41,41	0
32	MG	0	8013	1/1	0.06	-3.10	19,19,19,19	0
36	SR	1	8913	1/1	0.06	-3.11	108,108,108,108	0
32	MG	0	8031	1/1	0.07	-3.11	68,68,68,68	0
36	SR	0	8934	1/1	0.08	-3.22	138,138,138,138	0
34	NA	0	8520	1/1	0.07	-3.24	44,44,44,44	0
32	MG	0	8072	1/1	0.11	-3.27	45,45,45,45	0
36	SR	0	8902	1/1	0.10	-3.29	72,72,72,72	0
32	MG	0	8004	1/1	0.10	-3.31	19,19,19,19	0
32	MG	0	8021	1/1	0.07	-3.49	31,31,31,31	0
32	MG	0	8032	1/1	0.05	-3.53	47,47,47,47	0
32	MG	0	8075	1/1	0.07	-3.56	50,50,50,50	0
32	MG	0	8045	1/1	0.07	-3.63	28,28,28,28	0
36	SR	0	8910	1/1	0.11	-3.65	118,118,118,118	0
36	SR	0	8942	1/1	0.04	-3.68	123,123,123,123	0
36	SR	0	8978	1/1	0.07	-3.69	132,132,132,132	0
32	MG	0	8059	1/1	0.07	-3.81	55,55,55,55	0
32	MG	0	8025	1/1	0.04	-3.82	23,23,23,23	0
36	SR	0	8989	1/1	0.12	-3.92	174,174,174,174	0
37	CD	O	8705	1/1	0.04	-4.03	105,105,105,105	0
32	MG	0	8073	1/1	0.08	-4.12	89,89,89,89	0
36	SR	0	8949	1/1	0.09	-4.13	128,128,128,128	0
36	SR	0	8916	1/1	0.03	-4.17	110,110,110,110	0
36	SR	0	8945	1/1	0.05	-4.36	119,119,119,119	0
36	SR	0	8955	1/1	0.10	-4.47	200,200,200,200	0
32	MG	0	8087	1/1	0.07	-4.58	22,22,22,22	0
36	SR	0	8995	1/1	0.11	-4.62	123,123,123,123	0
32	MG	0	8006	1/1	0.09	-4.77	44,44,44,44	0
34	NA	0	8550	1/1	0.12	-4.86	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8018	1/1	0.07	-4.88	34,34,34,34	0
32	MG	0	8068	1/1	0.06	-4.92	44,44,44,44	0
32	MG	0	8024	1/1	0.03	-5.07	39,39,39,39	0
36	SR	0	8923	1/1	0.08	-5.09	108,108,108,108	0
32	MG	0	8042	1/1	0.05	-5.15	75,75,75,75	0
36	SR	B	8950	1/1	0.13	-5.23	123,123,123,123	0
32	MG	0	8007	1/1	0.09	-5.27	21,21,21,21	0
36	SR	0	8920	1/1	0.05	-5.37	145,145,145,145	0
36	SR	0	8966	1/1	0.05	-5.90	101,101,101,101	0
32	MG	0	8017	1/1	0.10	-6.01	28,28,28,28	0
32	MG	0	8046	1/1	0.06	-6.16	44,44,44,44	0
36	SR	0	8917	1/1	0.08	-6.65	111,111,111,111	0
36	SR	0	8962	1/1	0.05	-7.07	168,168,168,168	0
36	SR	0	8919	1/1	0.11	-7.60	185,185,185,185	0
36	SR	0	8927	1/1	0.09	-8.04	171,171,171,171	0
36	SR	0	9008	1/1	0.10	-8.75	94,94,94,94	0
32	MG	0	8092	1/1	0.05	-	53,53,53,53	0
36	SR	0	8997	1/1	0.83	-	200,200,200,200	0
36	SR	0	8973	1/1	0.16	-	142,142,142,142	0
36	SR	0	9006	1/1	0.32	-	200,200,200,200	0
32	MG	0	8091	1/1	0.16	-	67,67,67,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.